

10/190,887

(FILE 'HOME' ENTERED AT 12:33:42 ON 20 JAN 2005)

FILE 'REGISTRY' ENTERED AT 12:34:21 ON 20 JAN 2005

L1 STRUCTURE uploaded

=> d 11

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 12:35:04 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1335 TO ITERATE

74.9% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 24509 TO 28891

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 12:35:10 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 25918 TO ITERATE

100.0% PROCESSED 25918 ITERATIONS

70 ANSWERS

SEARCH TIME: 00.00.01

L3 70 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

FULL ESTIMATED COST

SESSION

161.97

FILE 'CAPLUS' ENTERED AT 12:35:17 ON 20 JAN 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 20 Jan 2005 VOL 142 ISS 4

FILE LAST UPDATED: 19 Jan 2005 (20050119/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 31 L3

=> d 1-31 bib abs

L4 ANSWER 1 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:550974 CAPLUS
DN 141:89551
TI Copolymers of ethylene with α -olefins
IN Mihan, Shahram; Lilge, Dieter
PA Basell Polyolefin G.m.b.H., Germany
SO PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 2004056878 | A2 | 20040708 | WO 2003-EP14437 | 20031218 |
| | WO 2004056878 | A3 | 20040923 | | |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| PRAI | DE 2002-10261252 | A | 20021220 | | |
| | US 2003-451836P | P | 20030304 | | |
| OS | MARPAT 141:89551 | | | | |
| AB | Copolymers of ethylene with α -olefins which have a molar mass distribution Mw/Mn of from 1 to 8, a d. of from 0.85 to 0.94 g/cm ³ , a molar mass Mn of from 10.000 g/mol to 4 000 000 g/mol and a CDBI of less than 50% and in which the side chain branching of the maxima of the individual peaks of the short chain branching distribution is in each case greater than 5 CH ₃ /1 000 carbon atoms, a process for preparing them, a catalyst suitable for preparing them and fibers, moldings, films or polymer mixts. in which these copolymers are present. | | | | |

L4 ANSWER 2 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:550904 CAPLUS
DN 141:89550
TI Preparation of chromium monocyclopentadienyl complexes useful as olefin polymerization catalysts
IN Mihan, Shahram; Nifant'ev, Ilya
PA Basell Polyolefine G.m.b.H., Germany
SO PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|------|----------|-----------------|----------|
| PI | WO 2004056482 | A1 | 20040708 | WO 2003-EP14447 | 20031218 |
| | | | | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
 PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
 TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 DE 10261109 A1 20040701 DE 2002-10261109 20021220
 PRAI DE 2002-10261109 A 20021220
 US 2003-490303P P 20030725
 OS MARPAT 141:89550
 AB Monocyclopentadienyl complexes in which the cyclopentadienyl system bears at least one unsubstituted, substituted or fused, heteroarom. ring system bound via a specific bridge, a catalyst system comprising at least one of the monocyclopentadienyl complexes, the use of the catalyst system for the polymerization or copolyrn. of olefins and a process for preparing polyolefins by polymerization or copolyrn. of olefins in the presence of the catalyst system and polymers obtainable in this way.
 RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT
 L4 ANSWER 3 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:550903 CAPLUS
 DN 141:89549
 TI Preparation of chromium monocyclopentadienyl complexes useful as olefin polymerization catalysts
 IN Mihan, Shahram; Enders, Markus; Nifant'ev, Ilya; Nicoara, Cristiana
 PA Basell Polyolefine G.m.b.H., Germany
 SO PCT Int. Appl., 68 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 3

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|------------------|----------|
| PI | WO 2004056481 | A1 | 20040708 | WO 2003-EP13748 | 20031205 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | DE 10261109 | A1 | 20040701 | DE 2002-10261109 | 20021220 |
| PRAI | DE 2002-10261109 | A | 20021220 | | |
| | US 2003-490303P | P | 20030725 | | |
| OS | MARPAT 141:89549 | | | | |
| AB | Monocyclopentadienyl complexes in which the cyclopentadienyl system bears at least one unsubstituted, substituted or fused, 5-membered heteroarom. ring system bound via a specific bridge, a catalyst system comprising at least one of the monocyclopentadienyl complexes, the use of the catalyst system for the polymerization or copolyrn. of olefins and a process for preparing polyolefins by polymerization or copolyrn. of olefins in the presence of the | | | | |

catalyst system and polymers obtainable in this way.
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:548478 CAPLUS
DN 141:243649
TI C6F5-Group Transfer from [MeB(C6F5)3]- to the Metal Center of L2MMet+ (M = Ti, Zr) as a Deactivation Pathway in Olefin Polymerization Catalysis: A Combined Density Functional Theory and Molecular Mechanics Investigation
AU Wondimagegn, Tebikie; Xu, Zhitao; Vanka, Kumar; Ziegler, Tom
CS Department of Chemistry, University of Calgary, Calgary, AB, T2N 1N4, Can.
SO Organometallics (2004), 23(16), 3847-3852
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
AB Rates of pentafluorophenyl group transfer from borate anion to metal center of titanium and zirconium potential catalysts of ethylene polymerization are comparable with the rates of the second insertion of ethylene at temps. above 100°, thus providing a pathway of catalyst deactivation. Activation energies of C6F5-group transfer from the MeB(C6F5)3 counterion were calculated for [CpM(N:PR3)MMe]+, [Cp(N:CR2)MMe]+, [Cp*(N:CR2)MMe]+, [(CpSiMe2NR)MMe]+, [(N:PR3)2MMe] and [Cp(OSiR3)MMe] + (M = Ti, Zr; R = tBu), being in the range of 17-29 kcal/mol for Ti complexes and of 6-11 kcal/mol for zirconium counterparts. Enthalpies of the reaction, calculated on the basis of optimized geometries of the products, [Cp(L)M(C6F5)Me]-MeB(C6F5)2, are in the range of -4 to -10 kcal/mol. This reaction, which produces L2MMe(C6F5) and MeB(C6F5)2, is a possible deactivation pathway in metal-catalyzed single-site olefin polymerization

With M

= Ti and Zr, the results show that aryl group transfer is more facile for zirconium catalysts than for the corresponding titanium systems. Furthermore, electron-donating ligands and sterically demanding substituents play a crucial role in preventing the aryl transfer reaction. The aryl group transfer is likely to take place for (Cp)(NCR2)MMe+ with both titanium- and zirconium-ketimide complexes at about 100°. However, the decomposition temperature is raised to 250° for the corresponding (η 5-C5Me5)(NCR2)TiMe+ system.

RE.CNT 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:525973 CAPLUS
DN 141:72043
TI Olefin polymerization catalysts based on monocyclopentadienyl complex systems
IN Mihan, Sharam; Nifant'ev, Ilya
PA Basell Polyolefine GmbH, Germany
SO Ger. Offen., 39 pp.
CODEN: GWXXBX
DT Patent
LA German

FAN.CNT 3

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|---|----------|------------------|----------|
| PI | DE 10261109 | A1 | 20040701 | DE 2002-10261109 | 20021220 |
| | WO 2004056481 | A1 | 20040708 | WO 2003-EP13748 | 20031205 |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, | | | |

PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
 TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 WO 2004056482 A1 20040708 WO 2003-EP14447 20031218
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
 PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
 TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 PRAI DE 2002-10261109 A 20021220
 US 2003-490303P P 20030725
 OS MARPAT 141:72043
 AB Monocyclopentadienyl complex, in which the cyclopentadienyl bears at least one unsubstituted, substituted or condensed heteroarom. ring system bound over a specific bridge, was used as catalysts for polymerization or copolymer.
 of olefins. Thus, ethylene was polymerized in the presence of 9.6 mg (3-(2-pyridyl-1-phenylmethyl)indenyl)chromium dichloride, MAO (Cr:Al = 1:500) and 10 mL hexene at 40° for 12 min to produce 8.7 g polyethylene having very high mol. weight of 238574 g/mol.
 L4 ANSWER 6 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:520133 CAPLUS
 DN 141:190902
 TI Synthesis of Main Group and Transition Metal Complexes with the (8-Quinolyl)cyclopentadienyl Ligand and Their Application in the Polymerization of Ethylene
 AU Enders, Markus; Kohl, Gerald; Pritzkow, Hans
 CS Anorganisch-Chemisches Institut der Universitat, Heidelberg, 69120, Germany
 SO Organometallics (2004), 23(16), 3832-3839
 CODEN: ORGND7; ISSN: 0276-7333
 PB American Chemical Society
 DT Journal
 LA English
 AB Sodium 8-quinolinyl cyclopentadienide, 8-quinolinyl-substituted trimethylsilyl cyclopentadiene derivative and chromium, titanium and aluminum 8-quinolinyl half-sandwich complexes were prepared and tested as catalysts of ethylene polymerization Nucleophilic addition of 8-lithioquinoline to the Cp₂Co⁺ cation gave η₄-(8-quinolinylcyclopentadiene)(η₅-cyclopentadienyl)cobalt(I) (7), which was oxidatively decomplexed by FeCl₃, liberating 8-quinolinyl-substituted cyclopentadiene (2a). Deprotonation by strong bases such as NaH or KH leads to the alkali metal quinolinyl cyclopentadienide salts, which were used in preparation of the corresponding Ti, Cr, and Al complexes. The chromium(III) complex [(8-C₉H₆N-κN)-η₅-C₅H₄]CrCl₂] 12 reacts with methylaluminoxane (MAO) to give a highly active catalyst for the polymerization of ethylene.
 RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT
 L4 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2003:864456 CAPLUS
 DN 140:111473

TI Synthesis and characterization of Zr(IV) and Y(III) complexes with monocyclopentadienyl ligands containing an additional site tethered by a coordinating 2,6-pyridine bridge. X-ray crystal structures of the zirconium complexes
AU Paolucci, Gino; Vignola, Manuela; Coletto, Luca; Pitteri, Bruno; Benetollo, Franco
CS Dipartimento di Chimica, Universita Ca' Foscari di Venezia, Venice, I-30123, Italy
SO Journal of Organometallic Chemistry (2003), 687(1), 161-170
CODEN: JORCAI; ISSN: 0022-328X
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 140:111473
AB A new monocyclopentadienyl ligand containing an addnl. site tethered by a coordinating 2,6-pyridine unit was prepared, rac-2-(1-hydroxy-2,2-dimethylpropyl)-6-[dimethyl(cyclopentadienyl)methyl]pyridine dilithium salt, LLi₂ (rac-4) that is analogous to the ligands present in cyclopentadienyl ligand containing an addnl. site tethered via a coordinating bridge (CGC). After reacting the dilithium salt of the ligand with ZrCl₄ in a molar ratio of 1:1 in THF the complex L₂ZrCl₂(THF) (rac-5) was obtained which forms an insol. oligomeric species after the loss of THF upon purification. From the mother liquor two crystalline species LH₂ZrCl₃ (rac-6) and LH₂ZrCl₄(THF) (rac-7) were isolated, whose x-ray crystal structures are reported. The reaction of LLi₂ with Y(OTf)₃ afforded the probably dimeric species [LYOTf]₂ (rac-8) from which [LY(CH₂SiMe₃)₂] (rac-9) was obtained after reaction with LiCH₂SiMe₃.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:864452 CAPLUS
DN 140:128719
TI Quinolyl-functionalized Cp-chromium polymerization catalysts: synthesis and crystal structures of alkylation products
AU Enders, Markus; Fernandez, Pablo; Mihan, Shahram; Pritzkow, Hans
CS Anorganisch-Chemisches Institut der Universitat, Heidelberg, 69120, Germany
SO Journal of Organometallic Chemistry (2003), 687(1), 125-130
CODEN: JORCAI; ISSN: 0022-328X
PB Elsevier Science B.V.
DT Journal
LA English
AB The quinolyl-functionalized Cp-chromium(III) complexes 1 and 2, which serve as precursors for highly active olefin polymerization catalysts, were alkylated with benzylmagnesium chloride. From these reactions, the new metal complexes 4, 5 and 6 were obtained and structurally characterized. The expected alkylchromium compound 4 is formed together with complex 5, where the nucleophile replaced a hydrogen atom at the quinoline substituent. The dinuclear complex 6 is formed by nucleophile addition, rearrangement and dimerization.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:242382 CAPLUS
DN 138:255651
TI Polymerization of olefins and polyolefins therefrom
IN Mihan, Shahram; Dorer, Birgit; Enders, Markus; Fernandez, Pablo
PA Basell Polyolefine G.m.b.H., Germany
SO PCT Int. Appl., 44 pp.

CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 2003025028 | A1 | 20030327 | WO 2002-EP10130 | 20020910 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | EP 1430088 | A1 | 20040623 | EP 2002-777054 | 20020910 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| | BR 2002012317 | A | 20040921 | BR 2002-12317 | 20020910 |
| | US 2004249095 | A1 | 20041209 | US 2004-489387 | 20040311 |
| PRAI | DE 2001-10145454 | A | 20010914 | | |
| | WO 2002-EP10130 | W | 20020910 | | |

OS MARPAT 138:255651

AB The invention relates to a method for the polymerization of olefins with the use

of catalyst containing a metal complex of groups 3, 4, 5, 6, 7, 8, 9, or 10 of the periodic table containing at least one group of the type C:NR1, C:PR1 (R1 = optionally halogenated C1-20 or organosilyl), C:O, C:S, or a heteroarom. ring system, containing at least one atom of groups N, P, O, or S. The invention also relates to polymers which can be obtained according to said method and to the use of said method for controlling the range of molar mass distribution. In an example, ethylene-1-hexene copolymer was produced using a catalyst based on 1-(8-quinolinyl)-2,3,4,5-tetramethylcyclopentadienylchromium dichloride, dimethylanilinium tetrakis(pentafluorophenyl)borate, iso-Bu3Al, and either BuLi or butyloctylmagnesium.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:242348 CAPLUS
DN 138:255648
TI Monocyclopentadienyl complexes with ring-condensed heterocycles as catalysts for ethylene polymerization
IN Mihan, Shahram; Nifant'ev, Ilya
PA Basell Polyolefine GmbH, Germany
SO PCT Int. Appl., 53 pp.

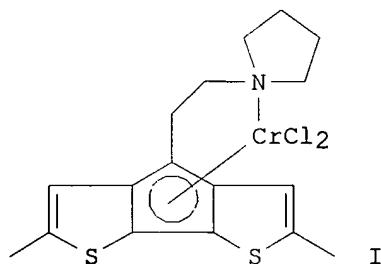
CODEN: PIXXD2

DT Patent
LA German

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|----------|
| PI | WO 2003024982 | A1 | 20030327 | WO 2002-EP10117 | 20020910 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW | | | | |

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
 CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 DE 10145453 A1 20030605 DE 2001-10145453 20010914
 EP 1425288 A1 20040609 EP 2002-777051 20020910
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
 BR 2002012520 A 20040824 BR 2002-12520 20020910
 US 2004242880 A1 20041202 US 2004-489023 20040309
PRAI DE 2001-10145453 A 20010914
 WO 2002-EP10117 W 20020910
 OS MARPAT 138:255648
 GI



AB Monocyclopentadienyl complex (HCp) YnM was prepared and used as ethylene polymerization catalyst, where HCp is a substituted cyclopentadienyl ring containing ≥ 1 condensed heterocycles, Y is a group attached on the cyclopentadienyl ring and comprises a neutral donor atom selected from Group 15-16 elements, M is a transition metal of Group 3-10 elements, and n = 1-3. Thus, ethylene was polymerized in the presence of 13.8 mg catalyst I-MAO-SiO₂ and 75 mg triisoprenylaluminum in heptane at 70°/40 bar for 60 min to yield 72 g polyethylene with an activity of 520 g PE/g cat.

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:132123 CAPLUS
DN 139:164564
TI Titanium dipyrrolylmethane derivatives: rapid intermolecular alkyne hydroamination
AU Shi, Yanhui; Hall, Christopher; Ciszewski, James T.; Cao, Changsheng; Odom, Aaron L.
CS Department of Chemistry, Michigan State University, East Lansing, MI, USA
SO Chemical Communications (Cambridge, United Kingdom) (2003), (5), 586-587
CODEN: CHCOFS; **ISSN**: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 139:164564
AB Alkynes are rapidly hydroaminated by primary amines using titanium dipyrrolylmethane derivs. as catalyst. The catalysts bis(N-methylmethanaminato)[2,2'-(1-methylethylidene)bis[1H-pyrrole]]titanium (I) and bis(N-methylmethanaminato)[2,2'-(1-propylbutylidene)bis[1H-pyrrole]]titanium (II) were reported. The I-catalyzed hydroamination of (1-propynyl)benzene with benzenamine gave N-(1-methyl-2-

phenylethyldiene)benzenamine in 83% yield. The mol. and crystal structures of II were reported.

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:516769 CAPLUS
DN 137:217024
TI Synthesis and Structure of Amino-Functionalized Cyclopentadienyl Vanadium Complexes and Evaluation of Their Butadiene Polymerization Behavior
AU Bradley, Sam; Camm, Kenneth D.; Furtado, Stephen J.; Gott, Andrew L.; McGowan, Patrick C.; Podesta, Thomas J.; Thornton-Pett, Mark
CS Department of Chemistry, University of Leeds, Leeds, LS2 9JT, UK
SO Organometallics (2002), 21(16), 3443-3453
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
OS CASREACT 137:217024
AB A number of bis-1,1,-amino-functionalized vanadocenes and vanadocene monochlorides were prepared; the bis-1,1,-amino-functionalized vanadocenes represent the first examples of structurally characterized compds. of this type, and the bis-1,1,-amino-functionalized vanadocene monochlorides represent the first examples synthesized and characterized. The catalytic behavior of some of the complexes toward butadiene is reported; and observe that amino-functionalized cyclopentadienyl vanadium phosphine chloride complexes behave much differently from their nonfunctionalized cyclopentadienyl derivs.

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:337510 CAPLUS
DN 137:155003
TI Reactions of pentafulvene complexes of titanium with nitriles and iso-nitriles - Synthesis and isomerizations of σ,π -chelate complexes with Cp.apprx.N-ligands
AU Stroot, J.; Saak, W.; Haase, D.; Beckhaus, R.
CS Fachbereich Chemie, Carl von Ossietzky Universitaet Oldenburg, Oldenburg, Germany
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (2002), 628(4), 755-761
CODEN: ZAACAB; ISSN: 0044-2313
PB Wiley-VCH Verlag GmbH
DT Journal
LA German
OS CASREACT 137:155003
AB The reactions of fulvene complexes $Cp^*Ti[\eta^6-C_5H_4:C(R)(R')]\text{Cl}$ [R = H, R' = CMe₃ (1); R = Me, R' = Me₂CH (4)] with nitriles and isonitriles, leading to σ,π -chelate complexes with Cp.apprx.N-ligands, were examined and the products formed characterized. Whereas in the reactions of 1 and 4 with nitriles a 1,2-mono-insertion of the CN-group into the Ti-C(R)(R') (Fv) bond is observed, the reaction with isonitriles leads to the insertion of two mols. of isonitrile. The nitrile insertion product of 1 was characterized by an imine-enamine tautomerization. Whereas the initially formed metastable imine species was only identified by NMR measurements in solution, the enamine tautomer $Cp^*Ti[\eta^5-C_5H_4C(CMe_3):C(C_6H_4Cl-4)NH:]\text{Cl}$ (2) crystallized from n-hexane, so that the crystal structure could be determined (space group P21/n, Z = 4, wR2 = 0.0897). In the reaction of 1 with 2,6-xylyl isonitrile (XyLNc), the initially formed iminoacyl complex rearranges due to the electrophilicity of the Ti center and builds a Ti-N bond with significant N(p π) \rightarrow Ti(d π)

bonding character in the product, $Cp^*Ti[\eta^5-C_5H_4CH(CMe_3)C(:C:NXyl)N(Xyl):]Cl$ (6), the structure of which was determined crystallog. (space group P.hivin.1, $Z = 2$, $wR_2 = 0.1216$).

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:923869 CAPLUS

DN 136:54205

TI Metallocene catalysts supported on calcined hydrotalcite for polymerization of olefins

IN Fraaije, Volker; Oberhoff, Markus; Huesgen, Nicola; Schopf, Markus; Bidell, Wolfgang; Wulff-Doering, Joachim; Mihan, Shahram

PA Basell Polyolefine G.m.b.H., Germany

SO PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|------------------|----------|
| PI | WO 2001096418 | A2 | 20011220 | WO 2001-EP6664 | 20010613 |
| | WO 2001096418 | A3 | 20020919 | | |
| | W: AU, BR, CA, CN, IN, JP, KR, PL, RU, SG, US, ZA RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR | | | | |
| | DE 10028432 | A1 | 20011220 | DE 2000-10028432 | 20000613 |
| | CA 2412333 | AA | 20021210 | CA 2001-2412333 | 20010613 |
| | EP 1290038 | A2 | 20030312 | EP 2001-955307 | 20010613 |
| | EP 1290038 | B1 | 20031203 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR | | | | |
| | BR 2001011589 | A | 20030506 | BR 2001-11589 | 20010613 |
| | AT 255601 | E | 20031215 | AT 2001-955307 | 20010613 |
| | JP 2004503622 | T2 | 20040205 | JP 2002-510553 | 20010613 |
| | ES 2211821 | T3 | 20040716 | ES 2001-1955307 | 20010613 |
| | ES 2211824 | T3 | 20040716 | ES 2001-1964972 | 20010613 |
| | US 2003176275 | A1 | 20030918 | US 2002-297996 | 20021212 |
| | ZA 2002010072 | A | 20031009 | ZA 2002-10072 | 20021212 |
| PRAI | DE 2000-10028432 | A | 20000613 | | |
| | WO 2001-EP6664 | W | 20010613 | | |

OS MARPAT 136:54205

AB The title catalysts, useful for polymerization of olefins, specifically ethylene

or propylene, and manufacture of polyolefins with reduced content of catalyst particle residues, comprise (A) calcined hydrotalcite, (B) ≥ 1 organotransition metal compound, e.g., dimethylsilylanyl bis(2-methylindenyl) zirconium dichloride (I), and (C) optionally ≥ 1 cation-forming compds., e.g., a linear or cyclic aluminoxane. For example, polymerization of propylene in the presence of $Al(CH_2CHMe_2)_3$ and

Puralox

MG 61 (calcined Al-Mg mixed oxide) which was treated with Me aluminoxane and I (procedure given), gave polypropylene (PP) particles with catalyst productivity 8300 g PP/g catalyst.

L4 ANSWER 15 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:923868 CAPLUS

DN 136:54204

TI Catalyst system for olefin polymerization comprising calcined hydrotalcite as catalyst support

IN Mihan, Shahram; Schopf, Markus; Fraaije, Volker; Oberhoff, Markus; Huesgen, Nicola; Bidell, Wolfgang; Wulff-Doering, Joachim

PA Basell Polyolefine G.m.b.H., Germany

SO PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|------------------|----------|
| PI | WO 2001096417 | A2 | 20011220 | WO 2001-EP6663 | 20010613 |
| | WO 2001096417 | A3 | 20020919 | | |
| | W: BR, CN, JP, KR, SG, US | | | | |
| | RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR | | | | |
| | DE 10028432 | A1 | 20011220 | DE 2000-10028432 | 20000613 |
| | EP 1290039 | A2 | 20030312 | EP 2001-964972 | 20010613 |
| | EP 1290039 | B1 | 20031203 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR | | | | |
| | BR 2001011583 | A | 20030506 | BR 2001-11583 | 20010613 |
| | AT 255602 | E | 20031215 | AT 2001-964972 | 20010613 |
| | JP 2004503621 | T2 | 20040205 | JP 2002-510552 | 20010613 |
| | ES 2211821 | T3 | 20040716 | ES 2001-1955307 | 20010613 |
| | ES 2211824 | T3 | 20040716 | ES 2001-1964972 | 20010613 |
| | ZA 2002010072 | A | 20031009 | ZA 2002-10072 | 20021212 |
| | US 2004033890 | A1 | 20040219 | US 2003-297998 | 20030606 |
| PRAI | DE 2000-10028432 | A | 20000613 | | |
| | WO 2001-EP6663 | W | 20010613 | | |

OS MARPAT 136:54204

AB A title system, useful for polymerization of olefins and manufacture of polyolefins

with reduced content of catalyst particle residues, comprises (A) calcined hydrotalcite, (B) ≥ 1 organotransition metal compound, (C) optionally ≥ 1 cation-forming compds., e.g., a linear or cyclic aluminoxane, and (D) ≥ 1 organomagnesium compound. For example, adding 18.6 mL of 4.75 M Me aluminoxane solution in PhMe to a suspension of 287.1 mg Eurecen 5031 in 4.1 mL PhMe, stirring the mixture for 45 min, combining the mixture with 14.2 g dried calcined Mg-Al oxide (Puralox MG 61), stirring the whole for 60 min and removing volatiles at ambient temperature and 10-3 bar gave 20.2 g of a yellowish beige solid. Adding 24.0 mg of the latter catalyst to a solution of 3 mL of butyloctylmagnesium (20% solution in heptane) in 400 mL isobutane under Ar in an autoclave, pressurizing the autoclave for 90 min with 40 bar ethylene and polymerizing at 70° gave 400 g polyethylene (PE) with viscosity 3.68 dL/g and productivity 16,670 g PE/g catalyst.

L4 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:886257 CAPLUS

DN 136:20354

TI Catalyst for the production of olefin polymers

IN Wang, Chunming

PA Union Carbide Chemicals & Plastics Technology Corp., USA

SO PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|----------|
| PI | WO 2001092346 | A2 | 20011206 | WO 2001-US12745 | 20010419 |
| | WO 2001092346 | A3 | 20020523 | | |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, | | | | |

LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, YU, ZA, ZW,
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
US 6723675 B1 20040420 US 2000-578273 20000525
US 2004171857 A1 20040902 US 2004-790887 20040301

PRAI US 2000-578273 A 20000525

OS MARPAT 136:20354

AB A catalyst composition for the polymerization of olefins is provided, comprising a cyclopentadienyl transition metal catalyst precursor and an activating co-catalyst. Thus, a catalyst system comprising (A) 5-[(2-pyridyl)methyl]1-1,2,3,4-tetramethylcyclopentadienylchromium(III) dichloride which was obtained by reacting 5-[(2-pyridyl)methyl]-1,2,3,4-tetramethylcyclopentadiene lithium (reaction product of tetramethylcyclopentadienyllithium, 2-picolyll chloride, and butyllithium) and chromium chloride tri(THF) and (B) MAO was placed in a stainless reactor with ethylene to give polyethylene.

L4 ANSWER 17 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:791509 CAPLUS

DN 136:263224

TI Synthesis and structure of ansa-cyclopentadienyl pyrrolyl titanium complexes: $[(\eta_5\text{-C}_5\text{H}_4)\text{CH}_2(2\text{-C}_4\text{H}_3\text{N})]\text{Ti}(\text{NMe}_2)_2$ and $[1,3\text{-}\{\text{CH}_2(2\text{-C}_4\text{H}_3\text{N})\}_2(\eta_5\text{-C}_5\text{H}_3)]\text{Ti}(\text{NMe}_2)$

AU Seo, Won Seok; Cho, Youn Jaung; Yoon, Sung Cheol; Park, Joon T.; Park, Younpong

CS Korea Advanced Institute of Science and Technology, Department of Chemistry and School of Molecular Science (BK21), Taejon, 305-701, S. Korea

SO Journal of Organometallic Chemistry (2001), 640(1-2), 79-84
CODEN: JORCAI; ISSN: 0022-328X

PB Elsevier Science S.A.

DT Journal

LA English

OS CASREACT 136:263224

AB Reaction of ansa-cyclopentadienyl pyrrolyl ligand $(\text{C}_5\text{H}_5)\text{CH}_2(2\text{-C}_4\text{H}_3\text{NH})$ (2) with $\text{Ti}(\text{NMe}_2)_4$ afforded bis(dimethylamido)titanium complex $[(\eta_5\text{-C}_5\text{H}_4)\text{CH}_2(2\text{-C}_4\text{H}_3\text{N})]\text{Ti}(\text{NMe}_2)_2$ (3) via amine elimination. A cyclopentadiene ligand with two pendant pyrrolyl arms, a mixture of 1,3- and 1,4- $\{\text{CH}_2(2\text{-C}_4\text{H}_3\text{NH})\}_2\text{C}_5\text{H}_4$ (4), underwent an analogous reaction with $\text{Ti}(\text{NMe}_2)_4$ giving $[1,3\text{-}\{\text{CH}_2(2\text{-C}_4\text{H}_3\text{N})\}_2(\eta_5\text{-C}_5\text{H}_3)]\text{Ti}(\text{NMe}_2)$ (5). Mol. structures of 3 and 5 have been determined by single crystal X-ray diffraction studies.

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:787139 CAPLUS

DN 136:85909

TI New Chromium(III) Complexes as Highly Active Catalysts for Olefin Polymerization

AU Enders, Markus; Fernandez, Pablo; Ludwig, Gunter; Pritzkow, Hans

CS Anorganisch-Chemisches Institut, Universitaet Heidelberg, Heidelberg, D-69120, Germany

SO Organometallics (2001), 20(24), 5005-5007

CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society

DT Journal

LA English

OS CASREACT 136:85909
AB Cyclopentadienyl ligands functionalized by quinoline or N,N-dimethylaniline have an ideal and rigid geometry for the formation of half-sandwich compds. As a result, stable chromium(III) complexes with intramol. nitrogen coordination have been obtained. Treatment with MAO leads to highly active, temperature-stable catalysts for the polymerization of ethylene.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:137265 CAPLUS
DN 134:193873
TI Copolymers of ethylene with C3-12- α -olefins, their production and their use
IN Mihan, Shahram; Lilge, Dieter; Schweier, Gunther; Enders, Markus
PA BASF Aktiengesellschaft, Germany
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | WO 2001012687 | A1 | 20010222 | WO 2000-EP7443 | 20000801 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2381723 | AA | 20010222 | CA 2000-2381723 | 20000801 |
| | BR 2000013271 | A | 20020416 | BR 2000-13271 | 20000801 |
| | EP 1204685 | A1 | 20020515 | EP 2000-958348 | 20000801 |
| | EP 1204685 | B1 | 20041013 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| | JP 2003507502 | T2 | 20030225 | JP 2001-517581 | 20000801 |
| | AU 773627 | B2 | 20040527 | AU 2000-69901 | 20000801 |
| | RU 2236420 | C2 | 20040920 | RU 2002-106424 | 20000801 |
| | AT 279455 | E | 20041015 | AT 2000-958348 | 20000801 |
| PRAI | DE 1999-19937863 | A | 19990813 | | |
| | WO 2000-EP7443 | W | 20000801 | | |

OS MARPAT 134:193873

AB Ethylene-C3-12- α -olefin copolymers with mol. weight distribution Mw/Mn \leq 10, d. 0.85-0.95 g/cm³, comonomer content 1-40 weight%, and number-average mol. weight Mn >150,000, and comonomer composition distribution breadth index >70%

are obtained by copolymer. in the presence of Cr complex catalysts. Examples were given for the preparation of dichloro[1-(8-quinolinyl)indenyl]chromium(III) and its use in the production of ethylene-1-hexene copolymer in the presence of Me aluminoxane.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:137225 CAPLUS
DN 134:178977
TI Monocyclopentadienyl complexes of chromium, molybdenum or tungsten with a

donor bridge
IN Mihan, Shahram; Lilge, Dieter; De Lange, Paulus; Schweier, Gunther;
Schneider, Martin; Rief, Ursula; Handrich, Udo; Hack, Johannes; Enders,
Markus; Ludwig, Gunter; Rudolph, Ralph

PA BASF Aktiengesellschaft, Germany

SO PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | WO 2001012641 | A1 | 20010222 | WO 2000-EP7442 | 20000801 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | US 6437161 | B1 | 20020820 | US 1999-373715 | 19990813 |
| | BR 2000013223 | A | 20020604 | BR 2000-13223 | 20000801 |
| | EP 1212333 | A1 | 20020612 | EP 2000-953135 | 20000801 |
| | EP 1212333 | B1 | 20030212 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| | AT 232539 | E | 20030215 | AT 2000-953135 | 20000801 |
| | JP 2003507387 | T2 | 20030225 | JP 2001-517539 | 20000801 |
| | EP 1288219 | A2 | 20030305 | EP 2002-26562 | 20000801 |
| | EP 1288219 | A3 | 20040102 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY | | | | |
| | ES 2192538 | T3 | 20031016 | ES 2000-953135 | 20000801 |
| | US 2003036658 | A1 | 20030220 | US 2002-166130 | 20020611 |
| | US 6699948 | B2 | 20040302 | | |
| | US 2003036662 | A1 | 20030220 | US 2002-166140 | 20020611 |
| | US 6787498 | B2 | 20040907 | | |
| | US 2003055267 | A1 | 20030320 | US 2002-166068 | 20020611 |
| | US 6838563 | B2 | 20050104 | | |
| PRAI | US 1999-373715 | A | 19990813 | | |
| | EP 2000-953135 | A3 | 20000801 | | |
| | WO 2000-EP7442 | W | 20000801 | | |

OS MARPAT 134:178977

AB The substituted monocyclopentadienyl, monoindenyl, monofluorenyl or heterocyclopentadienyl complexes of Cr, Mo or W (structures specified), wherein ≥ 1 of the substituents at the cyclopentadienyl ring carries a rigid donor function that is not exclusively linked via sp³ hybridized C or Si atoms, are useful as olefin (co)polymerization catalysts. The polyolefins

produced are useful for fibers, films and molded articles. For example, 1-indanone was condensed with lithiated 8-bromoquinoline in THF to give 1-(8-quinolyl)-1-indanol which was dehydrated by refluxing with HCl, the product 1-(8-quinolyl)indene was deprotonated with KH in THF and stirred with CrCl₃·3THF to give dichloro-[1-(8-quinolyl)indenyl]chromium(III) (I). Polymerization of ethylene in PhMe with Me aluminoxane-I catalytic system (Al:Cr ratio 1000:1) gave polyethylene having M_w 221,176 and M_w/M_n 47.3, with catalyst activity 3715 kg/molCr·h.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:48705 CAPLUS
 DN 132:222599
 TI Donor-Ligand-Substituted Cyclopentadienylchromium(III) Complexes: A New Class of Alkene Polymerization Catalyst. 1. Amino-Substituted Systems
 AU Doebring, A.; Goehre, J.; Jolly, P. W.; Kryger, B.; Rust, J.; Verhovnik, G. P. J.
 CS Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, D-45470, Germany
 SO Organometallics (2000), 19(4), 388-402
 CODEN: ORGND7; ISSN: 0276-7333
 PB American Chemical Society
 DT Journal
 LA English
 AB Me₂NC₂H₄C₅Me₄Li reacts with Cr(THF)₃Cl₃ to give ($\eta^1:\eta^5$ -Me₂NC₂H₄C₅Me₄)CrCl₂, in which the complexation of the N-donor atom to the metal atom has been confirmed by x-ray crystallog. A series of related compds., e.g. ($\eta^1:\eta^5$ -cyclo-C₄H₈NSiMe₂OSiMe₂C₅H₄)CrCl₂, has been prepared by varying the substituents on the organic ligand. Further reaction with organomagnesium reagents leads to formation of the corresponding dialkyl-Cr complexes. Related species have been prepared containing imine-, alkoxy-, and alkylthio-substituted cyclopentadienyl groups as well as the C-donor ligand tetramethylimidazol-2-ylidene. Treatment of these compds. with methylalumoxane (MAO) leads to the formation of highly active catalysts for the oligomerization, polymerization, and copolymerization of ethylene.
 RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1998:745061 CAPLUS
 DN 130:25453
 TI Bridged phosphole-cyclopentadienyl compounds, preparation of their metal complexes, and their use in polymerization of olefins
 IN Von Haken Spence, Rupert Edward; Gao, Xiaoliang; Koch, Linda; Brown, Stephen John; Harrison, Daryll G.; Wang, Qinyan
 PA Nova Chemicals (International) S.A., Switz.
 SO PCT Int. Appl., 44 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

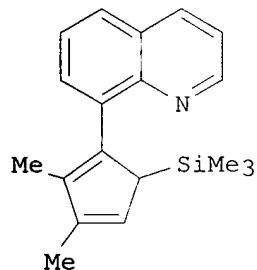
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 9850392 | A1 | 19981112 | WO 1998-CA428 | 19980501 |
| | W: AL, AM, AT, AU, AZ, BA, BG, BR, BY, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, JP, KE, KG, KP, KR, KZ, LK, LT, LV, MX, NO, NZ, PL, PT, RO, RU, SD, SG, SI, SK, TJ, TM, TR, UA, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2204803 | AA | 19981108 | CA 1997-2204803 | 19970508 |
| | US 6051667 | A | 20000418 | US 1998-65594 | 19980424 |
| | AU 9872024 | A1 | 19981127 | AU 1998-72024 | 19980501 |
| | EP 983280 | A1 | 20000308 | EP 1998-919010 | 19980501 |
| | EP 983280 | B1 | 20030205 | | |
| | R: AT, BE, DE, DK, ES, FR, GB, IT, NL, SE, FI | | | | |
| PRAI | CA 1997-2204803 | A | 19970508 | | |
| | WO 1998-CA428 | W | 19980501 | | |
| OS | MARPAT 130:25453 | | | | |
| AB | Phospholes having a metalloid bridge to a cyclopentadienyl group are | | | | |

prepared by reacting an organometallic cyclopentadienyl reagent with a phosphole bearing a halogen or pseudohalogen group. Group 4 metal complexes of these phospholes are excellent polymerization catalysts, especially for

the polymerization of olefins at high temperature. Thus, successive reaction of Cp₂ZrHCl (Cp = cyclopentadienyl) with MeC.tplbond.CMe, MeLi, MeC.tplbond.CSiMe₂Cl, and PhPCl₂ gave 2-(chlorodimethylsilyl)-3,4,5-trimethyl-1-phenylphosphole, which was treated with CpLi to give 2-(cyclopentadienyldimethylsilyl)-3,4,5-trimethyl-1-phenylphosphole (I). Successive treatment of I with Li foil, Me₃SnCl, and ZrCl₄ in THF gave a metallocene-like Zr complex, which was used with a modified Me aluminoxane for solution polymerization of ethylene in cyclohexane at 1500 psi.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:811879 CAPLUS
DN 128:115037
TI Chiral titanium and zirconium complexes with 1-(8-quinolyl)-2,3-dimethylcyclopentadienyl ligands
AU Enders, Markus; Rudolph, Ralph; Pritzkow, Hans
CS Im Neuenheimer Feld, Anorganisch-Chemisches Institut der Universitat, Heidelberg D-69120, 270, Germany
SO Journal of Organometallic Chemistry (1997), 549(1-2), 251-256
CODEN: JORCAI; ISSN: 0022-328X
PB Elsevier Science S.A.
DT Journal
LA German
OS CASREACT 128:115037
GI



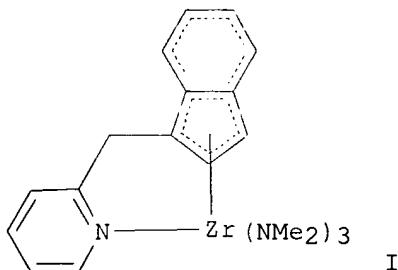
I

AB Reaction of 8-lithioquinoline with 2,3-dimethylcyclopent-2-en-1-one leads to 1-(8-quinolyl)-2,3-dimethylcyclopentadiene (1) after hydrolysis and H₂O elimination in acidic solution. With strong bases 1 is deprotonated to an intensively red-colored anion. The latter was converted to the trimethylsilyl derivative 3 (shown as I), which could be characterized by crystal structure anal. 3 Reacts with Group 4 transition metal chlorides to give the corresponding chiral trichlorotitanium and trichlorozirconium complexes 4 and 5. 4 Was examined by crystal structure anal. and shows the expected interaction between the quinolyl N atom and the metal center.

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:753748 CAPLUS
DN 128:115032
TI New chelating pyridyl-indenyl and quinolyl-indenyl ligands leading to C₁ symmetrical complexes of zirconium via amine elimination. X-ray structure

AU of [3-(2-pyridylmethyl)(indenyl)tris(dimethylamido)Zr(IV)
 Ziniuk, Zeev; Goldberg, Israel; Kol, Moshe
 CS Raymond and Beverly Sackler Faculty of Exact Sciences, School of
 Chemistry, Tel-Aviv University, Tel-Aviv 69978, Israel
 SO Journal of Organometallic Chemistry (1997), 545-546, 441-446
 CODEN: JORCAI; ISSN: 0022-328X
 PB Elsevier Science S.A.
 DT Journal
 LA English
 OS CASREACT 128:115032
 GI

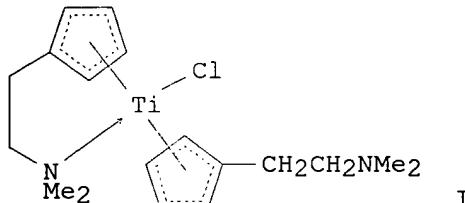


AB Two new chelating (1-) ligands, based on an indenyl group and either a pendant pyridylmethyl arm or a pendant quinolylmethyl arm were synthesized. The two ligands react cleanly with tetrakis(dimethylamido)zirconium by amine elimination reactions leading to complexes of C1 symmetry. The crystal structure of the pyridyl-indenyl zirconium complex I was determined Compound I ($C_{21}H_{30}N_4Zr$) crystallizes in the orthorhombic space group Pbca with $a = 9.588(1)$, $b = 14.858(12)$, $c = 29.932(7)$ Å, $V = 4264.1$ (A3), $Z = 8$. The structure refinement converged to $R_1 = 0.049$ for $2363 F_0 > 4\sigma(F_0)$ and $wR_2 = 0.167$ for all 3197 unique data, $S = 1.04$. The structure shows that the indenyl is bound in a η^5 fashion blocking the top of the zirconium atom, and the pyridine is coordinated in an exceptionally long $2.536(5)$ Å N-Zr bond, blocking the back of the zirconium atom.

L4 ANSWER 25 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1997:708438 CAPLUS
 DN 127:293336
 TI New Trigonal-Bipyramidal 5ansa-Zirconocene Derivatives. 1.
 {2,6-Bis(methylcyclopentadienyl)pyridine}zirconium(IV) Monochloride
 Monoalkyls and Dialkyls. Crystal Structure of $[Zr\{C_5H_3N(CH_2C_5H_4)_2-2,6\}(n-C_4H_9)_2]$, the First Thermally Stable Dialkylzirconocene Containing β -Hydrogens
 AU Paolucci, Gino; Pojana, Giulio; Zanon, Jacopo; Lucchini, Vittorio;
 Avtomonov, Evgeni
 CS Dipartimento di Chimica, Universita di Venezia, Venice, I-30123, Italy
 SO Organometallics (1997), 16(24), 5312-5320
 CODEN: ORGND7; ISSN: 0276-7333
 PB American Chemical Society
 DT Journal
 LA English
 AB The reaction of the new ligand $Na_2[2,6-(C_5H_4CH_2)_2C_5H_3N]$ (Na_2L) with $ZrCl_4$ in THF affords in good yield the trigonal-bipyramidal complex $LZrCl_2$, where the two Cl atoms are not equivalent. When $LZrCl_2$ and $RMgCl$ ($R = CH_3, Bu, CH_2SiMe_3$) are reacted in 1:1 and 1:2 molar ratios, the corresponding complexes $LZr(Cl)R$ and $LZrR_2$ can be isolated in good yields. Differently from the Cp_2ZrBu_2 , which has never been isolated due to β -H

elimination, the analogous L₂ZrBu₂ is thermally stable and its x-ray crystal structure was solved, confirming its trigonal-bipyramidal geometry with the alkyl groups occupying an equatorial and an axial position. An NMR study (¹H, ¹³C, HMQC, NOE) allowed the complete structural characterization of the complexes in solution

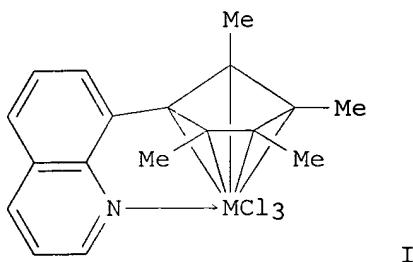
L4 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:720872 CAPLUS
DN 126:74988
TI Synthetic and structural studies on substituted cyclopentadienyl titanium(III) complexes with intramolecular amino group coordination
AU Qian, Yanlong; Guo, Rongwei; Huang, Jiling
CS Laboratory Organometallic Chemistry, East China Univ. Science Technology, Shanghai, 200237, Peop. Rep. China
SO Polyhedron (1996), Volume Date 1997, 16(1), 195-198
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier
DT Journal
LA English
OS CASREACT 126:74988
GI



AB Three substituted cyclopentadienyl Ti(III) complexes with intramol. amino group coordination were prepared and the crystal structure of (C₅H₄CH₂CH₂NMe₂)₂TiCl (1; shown as I) was determined

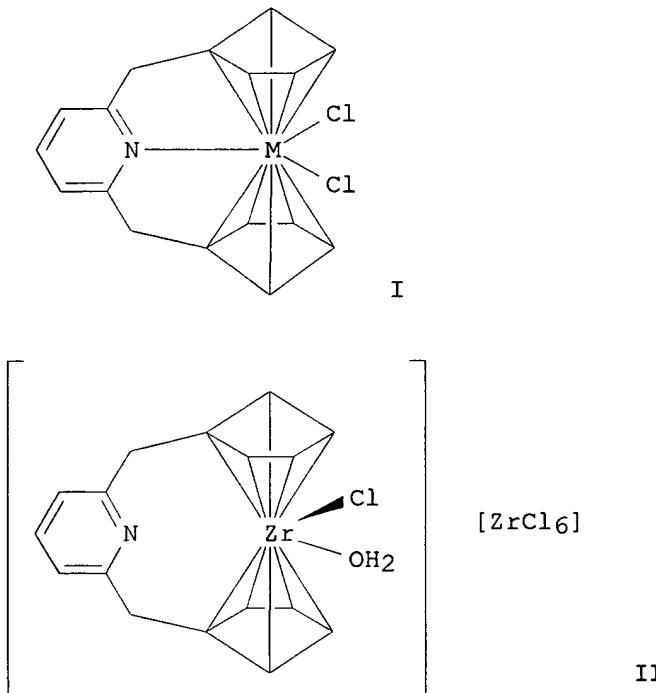
RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:190139 CAPLUS
DN 125:11011
TI 8-Quinolylcyclopentadienyl, a ligand with a tailored fit for chelate complexes
AU Enders, Markus; Rudolph, Ralph; Pritzkow, Hans
CS Anorg.-Chem. Inst., Univ. Heidelberg, Heidelberg, D-69120, Germany
SO Chemische Berichte (1996), 129(4), 459-63
CODEN: CHBEAM; ISSN: 0009-2940
PB VCH
DT Journal
LA English
GI



AB 2-R-8-lithioquinolines ($R = H, Me$) react with 2,3,4,5-tetramethylcyclopentenone to give the corresponding 2-R-8-quinolylcyclopentadienes after acidic workup and treatment with NH₃. Two of the possible 3 isomers are formed; the acidic protons on the Cp rings show unusual downfield shifts in the ¹H NMR spectra. Treatment with strong bases ($R = H$) led to the intensely colored anionic species which was converted into the trimethylsilyl derivative which is a suitable starting compound for the complexes I ($M = Ti, Zr$). The 2 complexes were investigated by crystal structure analyses. In both cases the quinolyl nitrogen atom is coordinated to the metal.

L4 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:638136 CAPLUS
DN 123:169761
TI 2,6-Bis(methylenecyclopentadienyl)-pyridine-zirconocene and -hafnocene dichloride; formation and crystal structure of [C₅H₃N-2,6-(CH₂-C₅H₄)₂Zr(Cl)(OH₂)]₂[ZrCl₆]
AU Thiele, K. H.; Schliessburg, Ch.; Neumueller, B.
CS Inst. Anorg. Chemie, Martin-Luther-Univ., Merseburg, Germany
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1995), 621(6), 1106-10
CODEN: ZAACAB; **ISSN**: 0044-2313
PB Barth
DT Journal
LA German
OS CASREACT 123:169761
GI



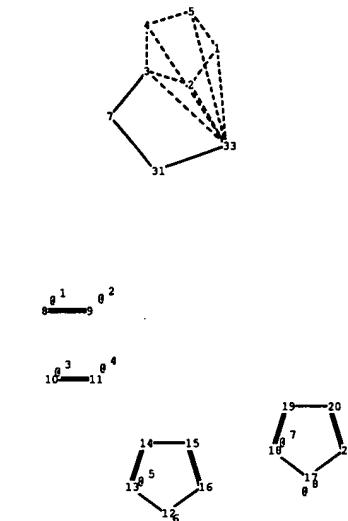
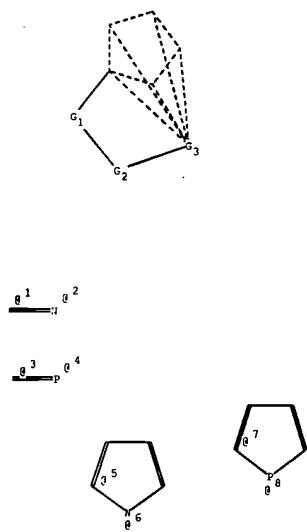
AB Pyridine bridged metallocene dichlorides I ($M = Zr, Hf$) were synthesized. The presence of $N \rightarrow Zr$ interaction favors the formation of zirconocene cations. Traces of water cause the formation of the salt-like compound II. The new compds. were characterized by 1H NMR, and mass spectroscopy. The x-ray crystal structure of II shows discrete cations and anions which are connected by H-bridges.

L4 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1994:217989 CAPLUS
 DN 120:217989
 TI Synthesis of 5-ansa-zirconocene complexes and crystal structure of $[Zr\{C_6H_4(CH_2C_5H_4)_2-1,3\}Cl_2]$
 AU Qian, Changtao; Guo, Jianhua; Ye, Changqing; Sun, Jie; Zheng, Peiju
 CS Lab. Organomet. Chem., Shanghai Inst. Org. Chem., Shanghai, 200032, Peop. Rep. China
 SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1993), (22), 3441-5
 CODEN: JCDTBI; ISSN: 0300-9246
 DT Journal
 LA English
 OS CASREACT 120:217989
 AB Zirconocene derivs. with interannular $MeN(CH_2CH_2)_2$, $C_5H_3N(CH_2)_2-2,6$ or $C_6H_4(CH_2)_2-1,3$ bridges were synthesized by the reaction of the corresponding disodium salts with $ZrCl_4$. The crystal structure of dichloro[m-phenylenedimethylenebis(η^5 -cyclopentadienyl)]zirconium was determined by x-ray crystallog.

L4 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1990:158486 CAPLUS
 DN 112:158486
 TI Synthesis of novel substituted cyclopentadienes and their early transition metal complexes
 AU Clark, T. Jeffrey; Nile, Terence A.; McPhail, Donald; McPhail, Andrew T.
 CS Dep. Chem., Univ. North Carolina, Greensboro, NC, 27412, USA
 SO Polyhedron (1989), 8(13-14), 1804-6

CODEN: PLYHDE; ISSN: 0277-5387
DT Journal
LA English
OS CASREACT 112:158486
AB Synthesis of two substituted cyclopentadienes, 1,3-bis(1-methylcyclohexyl)cyclopentadiene, Cp'H, and [2-methyl-2-(2-pyridyl)ethyl]cyclopentadiene, Cp''H, from fulvene intermediates is reported. These are readily converted to their early transition metal complexes Cp'W(CO)3Me, Cp''Mo(CO)3Me, Cp''W(CO)3Me, and [Cp''Ti(O)Cl·CH2Cl2]2. The x-ray crystal structure of the Ti compound shows that the N of the pyridine cyclopentadienyl substituent is coordinated to the Ti.

L4 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1987:176569 CAPLUS
DN 106:176569
TI Titanium hydride formation by hydrogen transfer from 2-methylpyridine to a titanium-fulvene compound; the first structurally characterized terminal titanium hydride
AU Pattiasina, Johannes W.; Van Bolhuis, Fre; Teuben, Jan H.
CS Dep. Chem., Univ. Groningen, Groningen, 9747 AG, Neth.
SO Angewandte Chemie (1987), 99(4), 342-3
CODEN: ANCEAD; ISSN: 0044-8249
DT Journal
LA German
OS CASREACT 106:176569
GI For diagram(s), see printed CA Issue.
AB Addition of 2-methylpyridine to Et2O solution of tetramethylfulvenetitanium complex I gave 45% titanium hydride complex II (R = H), the first complex of this type to be characterized. Reaction of II (R = H) with C2H4 and DCI gave II (R = Et, Cl), whereas, reaction of II (R = Et) with D gave II (R = D).



chain nodes :

8 9 10 11

ring nodes :

1 2 3 4 5 7 12 13 14 15 16 17 18 19 20 21 31 33

chain bonds :

8-9 10-11

ring bonds :

1-2 1-5 1-33 2-3 2-33 3-4 3-7 3-33 4-5 4-33 5-33 7-31 12-13
12-16 13-14 14-15 15-16 17-18 17-21 18-19 19-20 20-21 31-33

exact/norm bonds :

1-2 1-5 1-33 2-3 2-33 3-4 3-7 3-33 4-5 4-33 5-33 7-31 8-9
10-11 12-13 12-16 13-14 14-15 15-16 17-18 17-21 18-19 19-20
20-21 31-33

G1:C, Si, Ge, Sn

G2:[*1-*2], [*3-*4], [*5-*6], [*7-*8]

G3:Cr, Hf, Mo, Nb, Ti, V, W, Zr

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 31:Atom 33:Atom